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Summary report on CEA/DAM - CEA/DEN - LANL - IAEA - IPHC Collaboration Meeting on Nuclear Data, Nuclear Reaction Theories, and Machine Learning

Date and Location

Feb. 17 - 21, 2020, Bruyères-le-Châtel, France

List of Participants

CEA/DAM:

S. Hilaire, M. Dupuis, L. Batail, Y. Beaujeaurt-Teudiere, G. Blanchon,
P. Chau, N. Demeure, P. Dossantos-Uzarralde, N. Dubrey, N. Makaroff,
C. Pauline, N. Pillet, S. Peru, D. Regnier, P. Romain, C. De Saint-Jean, A.
Zdeb

CEA/DEN:

P. Tamagno

LANL:

T. Kawano, A. Lovell

IAEA:

R. Capote (remote)

IPHC (Institut Pluridisciplinaire Hubert Curien):

M. Kerveno (remote)

Introduction

Dupuis hosted our biennial CEA/NNSA collaboration meeting, and Kawano and Lovell of LANL and Tamagno of CEA/DEN (Cadarache) visited CEA/DAM to discuss current issues and further developments in nuclear reaction modeling, nuclear data evaluation, and relevant programs of modern computer science, especially the machine learning technology. The discussions included topics of our common interest such as neutron inelastic scattering, capture, and fission, with particular emphasis on the actinide nuclear data evaluations. We report briefly the summary of our discussions. We also had a half-day video meeting with Capote of IAEA and Kerveno of IPHC to discuss nuclear reactions on actinides.

Fission

A nuclear fission phenomenon is one of our main topics as the modeling of the dynamical process, and extracting relevant physical quantities those can be compared with observable data is still a big challenge in theoretical nuclear physics. We mainly discussed on our current modeling of the fission process and future plans, including the models for fission product yields, prompt fission neutron spectra, and fission cross sections.

Prompt fission decay

- We overviewed current methods to calculate fission product yield (FPY) after the prompt fission decay process; the Monte Carlo technique employed by FIFRELIN (CEA/DEN) and CGMF (LANL), and the deterministic model implemented in CoH₃ (LANL). An in-house version TALYS at IAEA now produces FPY by the deterministic method by reading pre-calculated data produced by CoH₃ or the SPY model at CEA/DAM.
- We also discussed the source code status. FIFRELIN is open now but in a binary format. CGMF will be an open source soon.
- To perform such prompt fission decay, some phenomenological inputs are essential. CEA is developing microscopic models to predict these data to reduce phenomenological assumptions. One example is the TD-BCS (time-dependent BCS) model to estimate how the total fission fragment excitation energy is shared by the two fragments. Such calculations are also performed by U. Washington and LANL by using TDHF (time-dependent Hartree-Fock).

Prompt fission neutron spectrum (PFNS)

- Capote reported a long-standing issue on the ²³⁵U(n,f) PFNS. Several dosimetry reaction cross sections, such as ²⁷Al(n,2n), are folded by the evaluated PFNS to obtain a spectrum averaged cross section, for which experimental data are available. For example, the average ²⁷Al(n,2n) cross section with the evaluation in JEFF gives 2.81 micro-barns, while the experimental value is 3.76 micro-barn.
- Such discrepancies are observed for reactions with high threshold energies, e.g. the (n,2n) reactions of ⁹⁰Zr, ⁵⁸Ni, ²³Na, ²⁷Al, etc. This indicates an issue in the high energy tail in PFNS when a Madland-Nix model at LANL or something similar models are adopted.
- The discrepancy increases when an aggregation technique used in the FPY calculation is used. Kawano presented a method to convert the evaporated neutron energies in the prompt fission decay process into the laboratory frame work, and discussed that the tail region should drop due to the reaction Q-values.
- We discussed this issue repeatedly, such as a possibility of scission neutrons, skewed excitation energy distribution in a fragment, etc. However, more detailed discussions will be needed to resolve this problem.

Dynamical fission process and cross section

- The fission path calculation with the HFB (Hartree-Fock-Bogoliubov) potential energy surface (PES), also as part of IAEA coordinated research project (CRP), on-going at CEA. The calculations for the even-even nuclei are almost done, and the odd nucleus cases are in progress with a new code. The 1-dimensional fission path results will be provided to IAEA CRP, although an exact schedule is not yet decided.
- LANL performs Langevin and/or random walk calculations on the semi-microscopic PES by the FRLDM (finite-range liquid drop model), and these data will be provided to users who study the fission process.

- The fission PES's both calculated microscopically and semi-microscopically should be compared carefully. This was planned before but not completed yet due to difference in the deformation coordinate employed in both models. A constrained local density HF calculation planned at CEA, which are already applied to fusion/fission calculations in the past, may help this exercise.
- In contrast to the original FRLDM, we now take more microscopic part in the model and calculate the local density with the single particle levels, since the shape parameterization Q_2 is different when the macroscopic part is taken.
- We discussed some issues in FRLDM, especially its stability; the Strutinsky method requires more careful attention to satisfy the so-called plateau condition. An updated parameterization and larger model space should be considered.
- As long-term objectives, we may implement a fission penetrability calculation in the Hauser-Feshbach nuclear reaction codes. A question of number of fission channels, which was also discussed at our previous meeting in 2018, still remains although.
- In addition to the LANL and CEA/DAM Hauser-Feshbach codes, CEA/DEN develops CONRAD that is also capable for fission cross section calculation. Such fission penetrability problem could be considered in CONRAD as well.

Photon strength function and neutron radiative capture reaction

- QRPA (quasi-particle random phase approximation) calculations at CEA still gives systematically 2-MeV higher peak-energies compared to the experimental data for both the E1 and M1 multipolarities. A Ph.D. student at CEA is trying to explain the 1 MeV shift in monopole states for Sn isotopes by looking at specific effective interaction properties as well as to the two-body center of mass correction in (Q)RPA. Coupling to four quasiparticle excitations may also contribute to those energy shifts and should be accounted for in the future.
- The calculated M1 strength spreads from low-energy to the pigmy resonance region, which seems to be consistent with experimental data. Although the new M1 table at CEA improves the calculated radiative capture cross sections, it was noted that a smooth connection between the observed up-bend at low energies and QRPA by analytical form could cause an artificial increase in the capture cross section.
- The nuclear level density is also an important quantity to calculate the capture cross section. It was reported that a temperature dependent level density improves prediction of the neutron average spacing D_0 . An effective interaction also plays an important role. At CEA, three forces, D1S, D1N, and D1M are employed, and D1M gives the best fit to nuclear masses.
- As alternative approach, we discussed the finite-amplitude method (FAM) developed by Nakatsukasa et al. CEA will be applying this technique to the HFB calculation, while LANL is planning to perform FAM for the FRDM single-particle wavefunctions.

Statistical model, direct and pre-equilibrium nuclear reaction models for neutron-induced reactions

General reaction theories

- Kawano presented some statistical properties of compound nucleus decay width by applying a GOE (Gaussian orthogonal ensemble) simulation. It was reported that isolated and strong-coupling regions show differences in calculated cross sections depending on how the decay widths are defined.
- Tamagno gave a talk on the R-matrix theory of nuclear reaction, and summarized recent R-matrix comparison study performed under the INDEN (International Nuclear Data Evaluation Network) collaboration at IAEA. The calculated cross sections with the available R-matrix codes give some differences, typically in the order of 0.1%, due to the Coulomb functions, relativistic kinematics, etc.

Direct reactions and optical potential

- In addition to a regular rotational band coupling scheme in the coupled-channels calculations, we introduce more coupling to the rotational levels build on top of the vibrational band-heads. This is very important for octupole band levels of actinides, which are strongly excited during the neutron-inelastic scattering process.
- For this purpose, optical potentials for the coupled-channels calculations and the multi-band coupling technique implemented in ECIS are discussed by comparing with the code OPTMAN developed by Soukhovitskii et al. Although the implementation in ECIS is not so clear, it seems OPTMAN includes higher order coupling terms than ECIS, which was also commented by Romain. This will be investigated more carefully in the near future.
- Since the coupling potential in ECIS is a macroscopic one, CEA replaces those by the transition matrix elements calculated by QRPA.
- Blanchon presented a new non-local optical potential solver, and announced that a paper will be published soon in CPC.
- Blanchon also presented a microscopic optical potential based on HFB + QRPA for Ca and Pb isotopes. It was reported that his technique works quite well for ^{40}Ca , but the ^{48}Ca case some issues. We discussed that there could have missing strength that determines the imaginary part in the optical potential, such as the compound nuclear reaction.

Pre-equilibrium and γ -ray production reactions

- We continued cross-checking of microscopically calculated $^{238}\text{U}(n,n')$ with JLM/QRPA at CEA and particle-hole excitations at LANL. We confirmed that the spin-transfer with both of the models is very similar. However, when plugged into the Hauser-Feshbach codes (TALYS at CEA, CoH₃ at LANL), we observed a significant difference in the inelastic scattering cross sections above 10 MeV.

- We suspected this is due to a method to mix the pre-equilibrium and compound spin population inside TALYS. We expect the γ -ray production for the 8^+ to 6^+ transition in $^{238}\text{U}(n,n')$ should be strongly suppressed as 1particle-1hole (or one phonon) state will be populated by a relatively small angular momentum transfer process. A farther check is needed to read the *preeqcorrect* subroutine in TALYS.
- Another origin of this difference may be related to the pre-equilibrium contribution at outgoing neutron energies above the incident energy minus neutron separation energy, which is larger within the JLM/QRPA approach.

(n,xn γ) data publication

- Kerveno summarized the $^{238}\text{U}(n, xn \gamma)$ data analysis status and publication plan. Our collaboration paper includes the measurement by IPHC, and model calculations by CEA, LANL, and IAEA. 18 γ -ray transitions for which we plan to include in the paper are already prepared, albeit some data still need to be corrected by a MCNPX simulation.
- A sensitivity analysis, presented at ND2019 in Beijing by Henning, will be included in the paper.
- In this paper, we focus on some selected γ -ray transitions, and discuss up-to-date nuclear reaction models to describe these transitions. A clear distinction will be made on the neutron inelastic scattering process;
 - The direct reaction that excites the low-lying levels,
 - the pre-equilibrium modeling and its spin distribution modify the γ -ray feeding from the continuum,
 - Engelbrecht-Weidenmueller transformation at low energies to deal the width fluctuation correction for deformed nuclei, and
 - Some discrete levels embedded in the continuum.
- It is important to avoid a code comparison. Although we understand the final goal is to estimate the total inelastic cross section that cannot be measured directly, we do not compare the total inelastic scattering in this paper. Such a paper will be produced separately, which focuses more on the application aspect.

Uncertainties and Machine Learning

Uncertainty quantification

- The Bayesian inference commonly used in the nuclear data evaluation gives the best estimate of the covariance, although it should be more conservative. Tamagno presented a method to create such a conservative covariance by splitting the parameter vector into the nuclear model parameters and experimental parameters, and apply a matrix (or analytical) marginalization, or a Bayesian (Monte Carlo) marginalization. He showed that the covariance matrices produced by these methods have larger diagonal elements.

- Tamagno also developed a technique to introduce a model defect in the uncertainty quantification, and applied to a simple model of ^{235}U PFNS. He demonstrated that one of the models (local model-defect method) increases the uncertainties in PFNS significantly.
- Demeure develops a C++ library to control computational numerical errors, such as truncation or round-off errors, to ensure accuracies in model calculations. In his development, an error is always associated with the value. This method will be applied to FELIX (finite element solver), SCAT2000 (C++ version of optical model code), and CONRAD.

Machine leaning

As increasing interest in applying the machine learning technique to nuclear physics, we devoted a half-day to discuss on this special subject, including three talks by Lovell, Makaroff, and Regnier.

- Lovell presented a machine leaning application to fission fragment yield prediction, where the mixture density network (MDN) is employed. The output, which is the fission yield, is represented by a sum of the normal Gaussian distributions, and the neural network learns the Gaussian variables. Interestingly the obtained average is different from a normal statistical analysis. We may need to add more physics constraints, such as the symmetry and normalization properties.
- The fission product yield model trained at a given energy-grid gives a reasonable interpolation between the points. However, the extrapolation violates the symmetric condition. The reason is still under investigation.
- Currently experimental data covariance is not taken into account. This will be included in future.
- Makaroff performed a meta-modelization of PES during his internship last summer at CEA. The deformation parameters Q_{20} , Q_{30} , Q_{40} data are the input to the neural network, and applied to the Gaussian process for HFB PES. This will be applied to estimate a starting value of the HF iteration for uncalculated PES.
- Regnier gave a brief introduction of history of neural network applications to nuclear masses, where experimental nuclear structure data - mass, radius, etc. - are the inputs. He constructed a five-dimensional collective Hamiltonian, and looked for the ground state in the calculated HFB states. Then he replaced HFB by the neural network, and trained it by the D1S HFB calculations. An example was shown for ^{178}Os , where the rotational states are well reproduced, while prediction of the vibrational states still needs improvement.

Others

We agreed to maintain this activity as this series of meeting benefits developments of theoretical nuclear physics at each laboratory. Although we do not have an explicit

schedule, this meeting was biennial in the past. There was a suggestion to make it annual, but we have not decided yet.